Poster I-7

Multiscale Simulations To Determine Structure-Function Relationships in Protein Ion Channels

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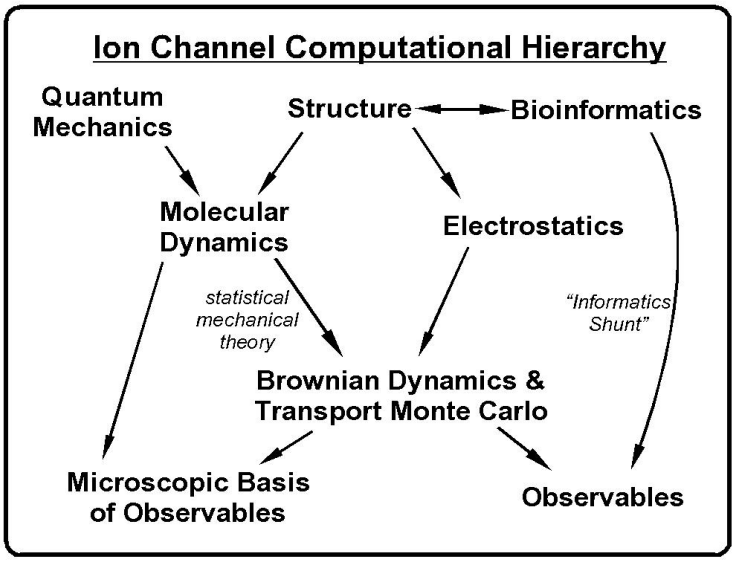
Even for a system as small as a small polypeptide, it is not feasible to do an *ab initio* simulation of dynamical properties for biologically relevant time scales of function. Therefore, in order to reliably and accurately infer the relationship between macromolecular structure and function, it is necessary to perform multiscale modeling and simulations. We have addressed this problem using protein ion channels as an exemplary system. The hierarchy of scales is shown in the figure below:



In this paper we present results from the application of this approach to gramicidin, porin, and potassium channels, discuss remaining algorithmic, theoretical, and software engineering problems, and describe Version 1.0 of the Ion Channel Simulator, an integrated multiscale simulation tool.

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